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1 Introduction

Radiation transport calculations are often used to estimate dose or exposure to components and personnel surrounding a radiation source. The sources for these calculations are decaying radionuclides within the various nuclear materials. Under long-term radiation exposure, some components may show signs of material damage such as hardening, cracking, discoloration, etc. resulting from the dose received from nearby radioactive sources. Radiation dose quantities are a useful means to correlate material damage or degradation to radiation interactions. The degradation is often dependent on how incident radiation interacts and deposits energy into the material. This dependence implies that radiation dose should be properly defined for the material effect of interest. Generic dose quantities, such as total energy deposited, may not necessarily correlate well for degradation of any given material.

Many of these material damage mechanisms have been studied and assigned dose thresholds that correspond to the silicon-equivalent dose in units of rad(Si) [1]. The purpose of this report is to discuss various methods to calculate silicon-equivalent dose and to provide suggestions for best practices. This report also includes a discussion of the application of the silicon-equivalent flux-to-dose conversion factors to non-silicon materials.

Silicon equivalent dose is often separated into two components: ionization and displacement dose. The silicon equivalent ionization and displacement doses may be summed for the total equivalent dose, without heating. The ionization dose component is the energy deposited through electronic interactions. Displacement dose is the energy deposited in the material from the neutron or photon interacting with the electrons surrounding the material nucleus and imparting energy. The displacement dose component captures the energy deposited in the material from a neutron or photon dislodging an atom from the molecular structure, thus creating an interstitial atom and vacancy pair [1].

This report uses an example scenario for illustration that consists of a stainless-steel vessel filled with various materials irradiated with ^{252}Cf point source neutrons located 25 cm away from the vessel. Only the neutron emission component of the ^{252}Cf point source is considered in this report. This report compares various ways of calculating silicon equivalent dose and compares two methods of applying flux-to-dose response functions with Monte Carlo N-particle Code (MCNP) [2]. MCNP is a Monte Carlo particle transport code developed at Los Alamos National Laboratory that has been validated for use in modeling a wide variety of radiation environments and in calculating dose [3, 4, 5, 6, 7, 8, 9]. The silicon equivalent dose response functions are defined to convert a neutron flux to a specific mode of energy deposition in silicon. The results section includes a discussion of the applicability of the silicon equivalent dose metric to materials that are exceedingly different in material makeup compared to pure silicon.

Neutron irradiation activates the stainless steel in the vessel. The activation gamma rays from the stainless steel vessel are considered as a source of potential dose to the fill material. The activation gamma rays from the stainless-steel is the only source of gamma dose evaluated in this report.

2 MCNP Model Details

This section discusses the details of the input deck used in the MCNP calculations used to estimate and to compare silicon equivalent doses. The section also discusses the assumptions made in the calculations. In order to estimate the dose to components for a radiation transport model, an input deck is required. The necessary parts for these models for simulation are a geometric model and material definitions, a source definition (radiation field), a tally definition (a record of the radiation interaction or energy deposited), and a response function for the tally. Section 2.1 details the geometry and materials used in the simulations. Section 2.2 discusses the source type and energy spectrum used in the MCNP calculations, and Section 2.3 includes a discussion of the tallies used in the MCNP calculations along with best practices. Section 2.3.2 shows the flux-to-dose response functions considered in this report. Section 2.4 discusses the setup and cross section data used to execute the transmutation calculation.

2.1 Geometry and Materials

The vessel used this example problem is model number 304L-05SF4-150 from Swagelok. An unstructured mesh representation of the CAD model shown in Figure 1, where the materials are called out and the overall dimensions are provided, is used in the MCNP model.

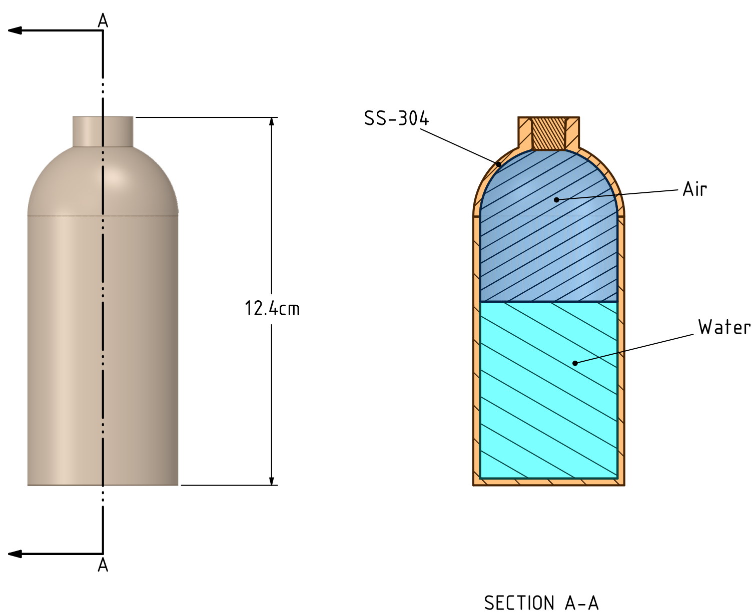

Figure 1: Overview of the CAD model of the vessel that was used to generate the unstructured mesh used in the MCNP calculations.

Swagelok provides computer-aided-drafting (CAD) files for most of their products including vessel 304-05SF4-150. The CAD file was imported into SpaceClaim (CAD software) [10] and needed no clean-up after import. Many models that are imported in to SpaceClaim for radiation transport applications have to be "cleaned-up" to repair overlaps, gaps, ill-defined surfaces, etc., and to remove irrelevant small CAD features such as very small fillets or holes. The vessel wall and cap are SS-304 and the vessel is filled to 150 ml with water, polyethylene, air, and stainless steel.

Attila4MC was used to import the CAD model and generate an unstructured mesh representation [11]. The mesh resolution parameters are chosen to properly represent the mass of the components in the model and not introduce a significant amount of error by over or under representing the mass of the components. Alwin et al. studied the sensitivities of selecting proper mass and volumetric meshing parameters and details the results in their report [12].

The air that fills the vessel and surrounds the vessel and source is dry air. All material isotopic compositions are from the PNNL-15870 Rev. 1 report [13] The point source is located 25 cm away from the center of the vessel and is located on plane with the center-of-mass of the vessel perpendicular to the vessel axis shown in Figure 1. Figure 2 shows a complete view of the entire model.

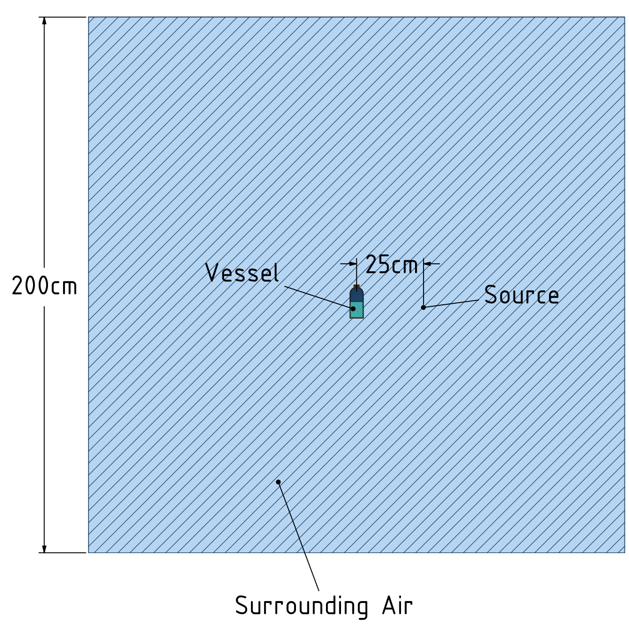

Figure 2: A two-dimensional overview of the MCNP model showing the various materials and dimensions.

2.2 Source Definition

The Cf-252 source is assumed to be a perfect spontaneous fission neutron source. The probability energy distribution of the neutron source used in the calculations is shown in Figure 3. The source is scaled to a source strength of 1×10^6 neutrons/sec and is implemented in the calculations as a point source. Equation 1 shows the Maxwellian Fission Spectrum equation, where $a = 1.18$, $b = 1.03419$, $p(E)$ is the probability function, E is energy in units of MeV, and C is a normalization constant.

$$p(E) = C \exp(-E/a) \sinh((bE)^{1/2}) \tag{1}$$

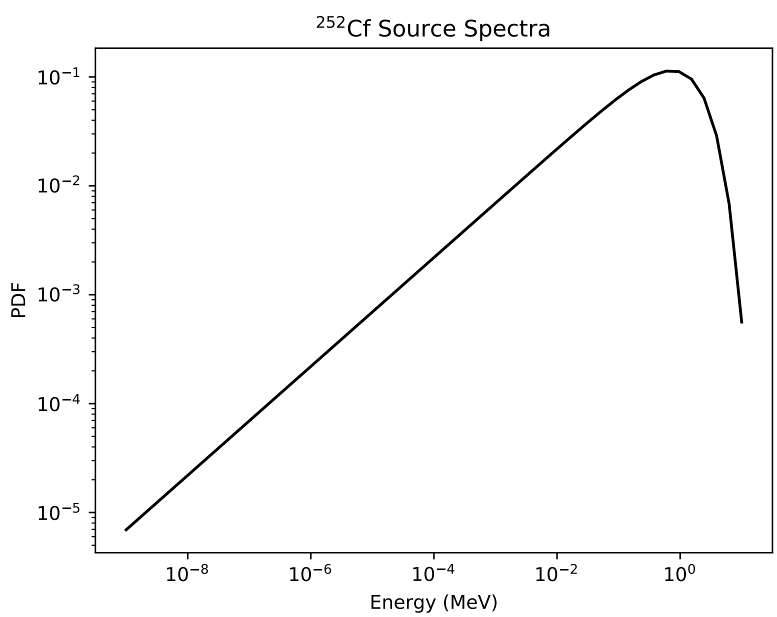

Figure 3: ^{252}Cf spontaneous fission neutron spectrum probability distribution used in these calculations. The distribution follows a Maxwellian Fission Spectrum equation where $a = 1.18$, $b = 1.03419$.

2.3 Tallies Definition

The input deck tally cards define how the radiation field and interactions should be recorded for further analysis. This section describes the tallies and the response functions applied in the tallies to estimate total silicon equivalent doses.

2.3.1 Dose

Dose in a given volume may be calculated a number of different ways in MCNP6. The `F6` energy deposition and the `+F6` collision heating tallies are ways to calculate the dose in the given material by tallying the energy deposited in the material in the cell volume. The main difference between the `F6` and `+F6` tallies is that the `+F6` tally tallies the energy deposited in the cell volume for all of the particle types listed on the mode card in the MCNP6 input deck, and the `F6` tally only tallies energy deposited by the specified particle designator when the tally is defined. One pitfall of using the `F6` tally is that an artificial factor of two may be introduced when tallying both photons and electrons on the same tally, or when adding individual particle tallies together. The `+F6` tally is the preferred method of calculating total energy deposition as opposed to summing individual `F6` tallies.

Dose to a material not in a model can be calculated with an `F4` volume-averaged flux tally with a `FM` tally multiplier card. The `FM` card specifies a series of constants where the user provides the ratio of the material in the cell to the material of interest, and specifies that the flux is to be multiplied by the density fraction as well as the atom density, total absorption cross section (for neutrons), and the average neutron heating number. The result of the `F4` tally with the `FM` card is in units of energy deposited per unit mass. One main assumption when calculating the energy deposition to a material not in the model is that the material does not significantly alter the neutron flux in the given cell volume. Another way to tally energy deposition in a material not in the model is to use the volume-averaged flux `F4` tally with either dose energy, `DE`, and dose function, `DF`, cards or energy bins, `E`, and energy multiplier, `EM`, cards to apply flux-to-dose conversion factors. The `DE` and `DF` cards should be applied if the flux-to-dose conversion factors are given in a point-wise fashion because the `DE` and `DF` cards interpolate (linearly by default) between the values provided in the `DE` and `DF` cards. The `E` and `EM` cards should be applied when the flux-to-dose conversion are provided in histograms.

2.3.2 Response Functions

Radiation interactions in a material are categorized by three general processes: displacing atoms, causing ionization, and heating the material [14]. The energy imparted to charged particles in the material is described by the kerma - kinetic energy released in matter [15]. The kerma may be divided into ionization kerma and into displacement kerma. The interaction mechanisms may correlate with observed damage in materials or components. Displacement kerma is a valid measure of performance degradation in bipolar transistors [15]. Whereas, for surface-effect devices, performance degradation is correlated with ionization kerma [15]. In the absence of detailed material degradation studies, total kerma should be considered as a metric for material degradation.

The total silicon equivalent dose is roughly the sum of the silicon ionization and displacement doses. Figure 4 shows the ionization and displacement components of the silicon equivalent dose response functions. The displacement dose response is from ASTM Standard E722-19 [15] and the ionization dose response is from ENDF B-VII [16]. For both the ionization and displacement dose response functions, dose response is highest toward high energies and minimizes near 10 eV. The functions clearly show local, sharp peaks from silicon cross-section resonances. These response functions are useful to correlate neutron fluence to damage in silicon, but may not be applicable to correlating damage in other materials. Ideally, a material-specific equivalent-dose response function should be used to correlate dose with kerma and degradation.

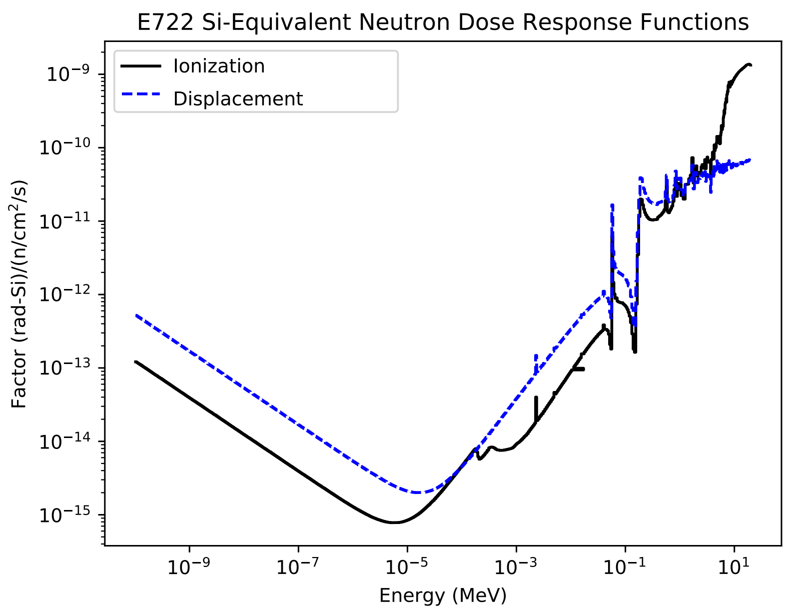

Figure 4: The ASTM Standard E722-19 silicon equivalent neutron displacement dose response function and ionization dose response. The responses are applied to the neutron flux to estimate energy deposition by displacement and by ionization.

ASTM Standard E722-19 describes the natural silicon displacement damage function in Appendix A of the standards and provides a conversion factor of 3.435×10^{-13} (rad(Si)$\cdot$cm^2)/(MeV$\cdot$mbarn), to convert the damage function to rad(Si)$\cdot$cm^2. ASTM Standard E722-19 also provides a conversion factor, 95 MeV$\cdot$mbarn, to convert the silicon damage function to 1-MeV silicon equivalent flux. To evaluate results from irradiations with different sources, the 1-MeV silicon-equivalent neutron dose reduces the neutron fluence from a source to a single parameter (an equivalent mono-energetic neutron source) applicable to a semiconductor material. The 1-MeV silicon equivalent flux assumes a specific damage correlation with neutron fluence. The 1-MeV silicon equivalent flux response function from E722-19 is shown in Figure 5. The user may easily convert from silicon equivalent displacement dose to 1-MeV silicon equivalent using the factors described above.

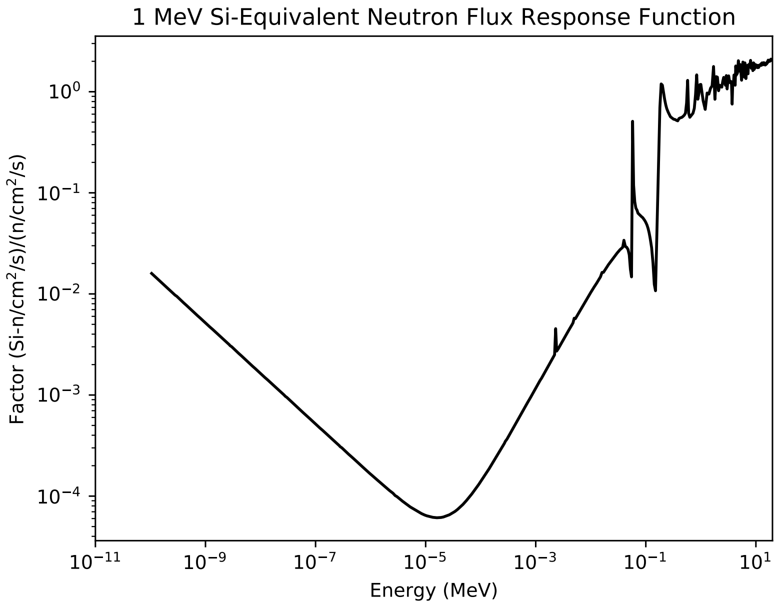

Figure 5: ASTM Standard E722-19 1-MeV silicon equivalent neutron flux response function used to reduce incident neutron fluence to a single parameter.

2.4 Activation Calculation Details

Activation of the stainless-steel vessel is calculated in MCNP to estimate activation gamma-ray dose to the fill material. The ^{252}Cf point source located 25 cm from the center of the water in the stainless-steel vessel is exposed to the vessel for an equivalent time of 41.5 hours. The calculation used the routines from the ACTIUM Python Toolkit to construct the CINDER2008 input files and generate the sdef card detailing the decay-gamma spectra at time steps following the initial activation period [17, 18]. CINDER2008 is a transmutation solver that assumes a constant neutron flux for the given volume and calculates the activation and transmutation of the nuclides defined in the material definition. The model was divided into regions that would assure a constant flux through the regions. The fluxes calculated with MCNP6 Version 6.2.1 are tallied in the same energy bin structure as the energy-group cross sections used by CINDER2008 and used as input in the CINDER2008 solver. The CINDER2008 cross section set has a 66 energy-group structure and consists of grouped cross sections from ENDF/B-VIII.0, JENDL4, and TENDL2017 in order of preference. The resulting decay-gamma energy spectrum at the end of the 41.5-hour irradiation period is used to calculate the equivalent dose in tissue throughout the model. The ICRP-57 photon dose response function is applied to the tallied photon flux to produce results in mrem/hour.

3 Results

This section contains details on calculating the silicon equivalent dose in the vessel fill materials. Section 3.1 shows the results relating to calculating the silicon-equivalent dose. Section 3.2 discussing the findings associated with the activation of the stainless steel in the vessel.

3.1 Silicon Equivalent Dose Rate Results

Dose rates were estimated with MCNP for a variety of vessel fill materials and are compared. Silicon equivalent dose was calculated with a variety of tallies as discussed in Section 2.3. Table 1 shows the results of calculating total silicon equivalent dose with `E` and `EM` cards. The total silicon flux is the sum of the silicon equivalent ionization dose and the silicon equivalent displacement dose. The %-Difference column in Table 1 compares the results from the response functions to a `+F6` collision heating tally on the silicon fill material where the mode card in the MCNP6 input deck included neutrons, photons, and electrons. The value of this collision heating tally is $(1.2851\pm0.0004)\times10^{-8}$ rad(Si)/s. The author chooses the `+F6` tally result in silicon the standard to which all other values of total silicon equivalent dose compare. The `+F6` tally includes all energy deposition contributions from all particles listed on the mode card in the MCNP input deck.

Table 1 shows that applying the dose response functions to tallies on materials other than silicon can introduce significant differences in the estimated silicon equivalent dose. Comparing the response function calculated value for silicon and the energy deposition tally value yield a 5% difference between the values. The neutron flux in each material is slightly different leading to slightly different total silicon equivalent dose for each material. The air-filled vessel has the best agreement with silicon heating dose from the `+F6` tally because the air minimally altered the neutron flux field. The total silicon equivalent dose estimate for the silicon fill differs from the `+F6` tally result because the `+F6` result includes some phonon heating that would not be included in the ionization and displacement flux-to-dose conversion factors. Additionally, the flux field is slightly affected through the vessel volume, thereby breaking the flux-to-dose conversion assumption of a uniform field. Errors shown in Table 1 are only statistical and do not quantify the systematic error in the calculations.

The use of `E` and `EM` or of `DE` and `DF` cards with the same flux-to-dose conversion factor can introduce error to the tally, if the origins of the flux-to-dose conversion factors are not known. The `E` and `EM` cards apply the flux-to-dose conversion factors in a histogram fashion. The pointwise `DE` and `DF` card input used for the flux-to-dose conversion factors are applied with logarithmic interpolation between the provided points. Table 2 shows the differences between applying `E` and `EM` or `DE` and `DF` cards when calculating silicon equivalent dose or 1-MeV silicon equivalent flux. The silicon equivalent flux-to-dose conversion factors given by ASTM Standard E722-19 are provided in a histogram format. The error introduced by the use of either the `E` and `EM` or `DE` and `DF` card can easily be avoided by understanding the original format of the flux-to-dose conversion factors.

Table 1: Silicon Equivalent Dose Rate Comparison in Variety of Vessel Fill Materials.

Material	Total Silicon Equivalent Dose[1] (rad(Si)/s)	%-Difference to Silicon +F6 [2]
Silicon +F6	$(1.2851\pm0.0004)\times10^{-8}$	-
Silicon	$(1.2197\pm0.0004)\times10^{-8}$	5.1%
SS-304	$(1.1718\pm0.0004)\times10^{-8}$	8.8%
Polyethylene	$(1.0267\pm0.0005)\times10^{-8}$	17%
Water	$(1.0639\pm0.0005)\times10^{-8}$	20%
Air	$(1.2398\pm0.0006)\times10^{-8}$	3.5%

[1] Tallied with a volume-averaged flux tally with response functions
[2] %-Difference =((+F6 Silicon Tally Result)- (Total Dose))/(+F6 Silicon Tally Result)×100

Table 2: E/EM vs. DE/DF Silicon Equivalent Dose Rate Comparison in Water

	E/EM Cards	DE/DF Cards	%-Difference[1]
Ionization Dose (rad(Si)/s)	$(6.704\pm0.003)\times10^{-9}$	$(6.52\pm0.02)\times10^{-9}$	2.7%
Displacement Dose (rad(Si)/s)	$(3.9350\pm0.0008)\times10^{-9}$	$(3.886\pm0.007)\times10^{-9}$	1.3%
1-MeV Equivalent Flux (n/cm^2/s)	$(1.2059\pm0.0002)\times10^{2}$	$(1.191\pm0.002)\times10^{2}$	1.2%

[1] (E/EM-DE/DF)/(E/EM)×100

Total silicon equivalent dose may also be calculated with a volume-averaged flux tally and a tally multiplier that substitutes silicon for the polyethylene material in the tally volume. Figure 6 shows a comparison of silicon equivalent dose tallied with a volume-averaged flux tally modified by a tally multiplier and modified with response functions applied with E/EM cards. The Response Calculated data, shown in Figure 6, are a sum of the ionization and displacement silicon equivalent dose. Overall, the two spectra in Figure 6 agree, except the energy integrated dose rate for the response calculated spectra is 5% higher than the FM calculated energy integrated dose.

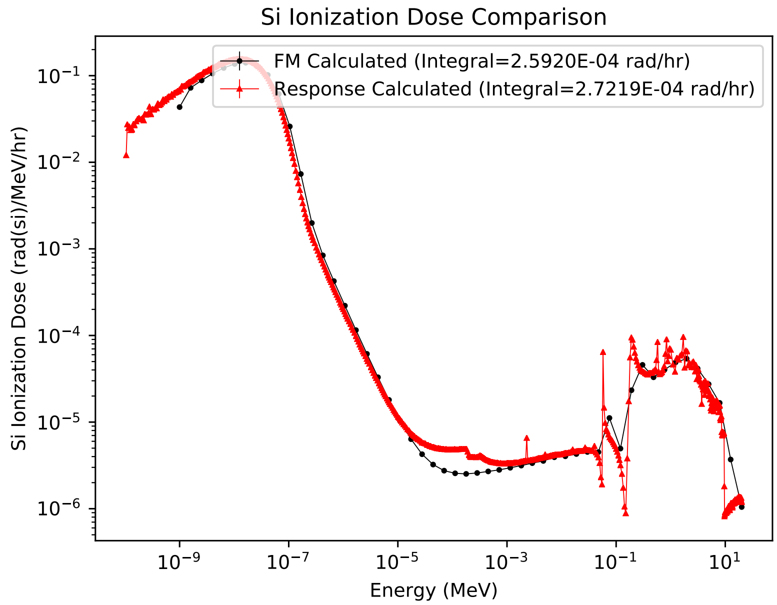

Figure 6: Silicon equivalent ionization dose in polyethylene calculated with a volume-average flux tally with a tally multiplier and with flux-to-dose conversion factors applied to the tally.

3.2 Activation Results

Figure 7 shows the equivalent decay-photon dose rate after a 41.5-hour irradiation with a ^{252}Cf neutron-spectrum point source with activity of 1×10^6 neutrons/sec. The total activity of the SS-304 vessel is 0.62 Bq where ^{56}Mn and ^{52}V make up 77% and 10%, respectively, of the total activity at the end of the irradiation period of 41.5 hours. The activation gamma-ray dose is negligible to the fill material and to personnel near the vessel and is below measurable limits for common radiation protection instruments.

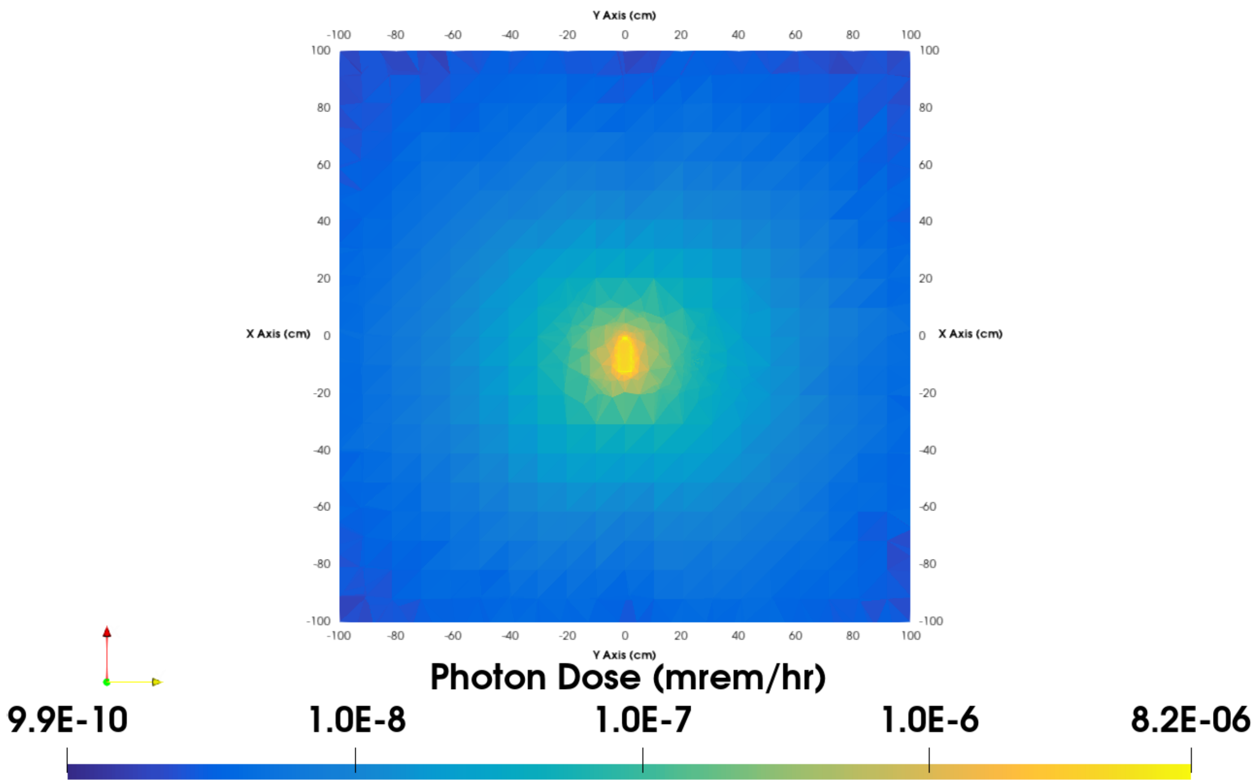

Figure 7: Equivalent photon dose rate for the activated SS-304 vessel exposed to a 1E6 n/s ^{252}Cf point source for 41.5 hours at the end of the irradiation period

4 Conclusions

Silicon equivalent dose is calculated in the material filling the inside of a stainless-steel vessel to demonstrate a number of approaches to calculate the dose in MCNP6. When comparing computational methods, the air material with the flux-to-dose conversion factors agreed best with the energy deposition tally in silicon because that fill altered the flux the least. Ideally, a material-specific equivalent dose response function should be used to correlate dose with kerma and degradation. The volume average flux tally modified by the tally multiplication card used to substitute the silicon material in the tallied volume favorably compares to a tally modified with flux-to-dose response functions. The flux-to-dose conversion factors from ASTM Standard E722-19 and ENDF B-VII were applied with both `E/ EM` and `DE/ DF` cards to highlight the errors introduced by applying the wrong data cards for the response functions. The user should expect errors of $\sim$1.5% when using the wrong `E/ EM` or `DE/ DF` card. The activation of the vessel is negligible for the given source strength and irradiation time.

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